20

chain nodes :

1 2 3 4 5 6 7 8 9 10 11 13 14 18 19 20 22 23 24 ring/chain nodes : 21

chain bonds :

1-11 1-2 1-22 2-3 2-9 3-4 3-7 4-5 5-6 6-8 6-13 9-10 13-14 18-21 18-19 18-20 23-24

exact/norm bonds :

1-2 1-22 3-7 5-6 6-8 13-14 18-21 18-19 18-20 23-24

exact bonds :

1-11 2-3 2-9 3-4 4-5 6-13 9-10

G1:C,O,S,Cb,Cy,Hy,N

G2:C,O

G3:[*1],[*2]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 13:CLASS 14:CLASS 18:CLASS 19:CLASS

20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

ANSWER 1 OF 36 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER:

1999:152298 CAPLUS

DOCUMENT NUMBER:

130:182770

TITLE:

Preparation of (N-substituted)-2-indolyl dipeptides

as

inhibitors of the ICE/ced-3 family of cysteine

proteases

INVENTOR(S):

Karanewsky, Donald S.; Bai, Xu

PATENT ASSIGNEE(S):

SOURCE:

U.S., 27 pp., Cont.-in-part of U.S. Ser. No. 767,175.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
US 5877197	A	19990302	US 1997-928989	19970912			
US 5869519	A	19990209	US 1996-767175	19961216			
CIORITY APPLN. INFO	. :		US 1996-767175	19961216			

PRI OTHER SOURCE(S):

MARPAT 130:182770

204919-40-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (N-substituted) indolyl dipeptides as inhibitors of the interleukin-1.beta. converting enzyme and related proteases)

204919-40-4 CAPLUS RN

Benzoic acid, 2,6-dichloro-,

4-carboxy-3-[[(2S)-2-[[(1,3-dimethyl-1H-indol-

2-y1)carbonyl]amino]-3-methyl-1-oxobutyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CAPLUS COPYRIGHT 1999 ACS ANSWER 2 OF 36

ACCESSION NUMBER:

1999:136764 CAPLUS

DOCUMENT NUMBER:

130:196957

TITLE:

Preparation of bicyclic peptide derivatives as interleukin-1.beta. converting enzyme inhibitors Batchelor, Mark James; Bebbington, David; Bemis, Guy

INVENTOR(S):

W.; Fridman, Wolf Herman; Gillespie, Roger John; Golec, Julian M. C.; Lauffer, David J.; Livingston,

David J.; Matharu, Saroop Singh; Mullican, Michael D.; Murcko, Mark A.; Murdoch, Robert; Zelle, Robert E. Vertex Pharmaceuticals Incorporated, USA PATENT ASSIGNEE(S): U.S., 189 pp., Cont.-in-part of U.S. Ser. No. SOURCE: 575,641. CODEN: USXXAM DOCUMENT TYPE: Patent English LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE ______ 19960208 19990223 US 1996-598332 US 5874424 Α WO 1996-US20843 19961220 A2 19970626 WO 9722619 A3 19971016 WO 9722619 W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG A1 19970714 AU 1997-15222 19961220 AU 9715222 EP 1996-945318 19981014 19961220 A2 EP 869967 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO NO 1998-2597 19980605 NO 9802597 19980812 Α US 1995-575641 19951220 PRIORITY APPLN. INFO .: US 1996-598332 19960208 US 1996-712878 19960912 US 1996-31495 19961126 US 1996-761483 19961206 WO 1996-US20843 19961220 MARPAT 130:196957 OTHER SOURCE(S): 175209-21-9P 175209-22-0P 175209-83-3P 192757-64-5P RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of bicyclic peptide derivs. as interleukin-1.beta. converting enzyme inhibitors) RN 175209-21-9 CAPLUS Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[[2-oxo-3-CN [[(phenylmethoxy)carbonyl]amino]-1(2H)-pyridinyl]acetyl]amino]butyl ester

Absolute stereochemistry. Rotation (-).

(9CI) (CA INDEX NAME)

175209-22-0 CAPLUS RN

Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[[2-oxo-3-[(1-oxo-3-CN phenylpropyl) amino]-6-(phenylmethyl)-1(2H)-pyridinyl]acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

175209-83-3 CAPLUS RN

Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[[(3S)-2,3,4,5-CN

tetrahydro-2-oxo-5-(1-oxo-3-phenylpropyl)-3-[(1-oxo-3-phenylpropyl)amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

RN 192757-64-5 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(3S)-3-(benzoylamino)-2,3,4,5-tetrahydro-5-(methylsulfonyl)-2-oxo-1H-1,5-benzodiazepin-1-yl]acetyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 3 OF 36 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1999:59441 CAPLUS

DOCUMENT NUMBER: 130:261459

TITLE: Three-Dimensional Quantitative Structure-Activity

Relationship of Interleukin 1-.beta. Converting

Enzyme

Inhibitors: A Comparative Molecular Field Analysis

Study

AUTHOR(S): Kulkarni, Santosh S.; Kulkarni, Vithal M.

CORPORATE SOURCE: Department of Chemical Technology Pharmaceutical

Division, University of Mumbai, Mumbai, 400 019,

India SOURCE:

J. Med. Chem. (1999), 42(3), 373-380

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal English

LANGUAGE: 151272-16-1 151272-17-2 153088-74-5 ΙT 154674-81-4 154674-82-5 154674-84-7 154674-86-9 173305-25-4 173305-41-4

205324-41-0 222406-86-2 222406-88-4 222406-90-8 222406-92-0 222406-93-1

222406-94-2 222406-96-4

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (QSAR of interleukin 1.beta. converting enzyme inhibitors: comparative mol. field anal. study)

151272-16-1 CAPLUS RN

L-Alaninamide, N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-3-[[2,6-1]])CN bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

151272-17-2 CAPLUS RN

L-Alaninamide, N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-3-(benzoyloxy)-1-CN (carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153088-74-5 CAPLUS

Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[(2S)-3-methyl-1-oxo-2-CN

[[(phenylmethoxy)carbonyl]amino]butyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 154674-81-4 CAPLUS

CN L-Alaninamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

__ OH

RN 154674-82-5 CAPLUS

CN L-Alaninamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

∕ он

RN 154674-84-7 CAPLUS

CN L-Alaninamide,

N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dihydroxybenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 154674-86-9 CAPLUS

CN L-Alaninamide,

N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

RN 173305-25-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-,

(3S)-4-carboxy-3-[[[2-(4-fluorophenyl)-6-oxo-5-[[(phenylmethoxy)carbonyl]amino]-1(6H)-pyrimidinyl]acetyl]amino]-2oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 173305-41-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[[6-oxo-5-[[(phenylmethoxy)carbonyl]amino]-2-(2-thienyl)-1(6H)-pyrimidinyl]acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

RN 205324-41-0 CAPLUS

CN L-Alaninamide,

Absolute stereochemistry.

RN 222406-86-2 CAPLUS

CN L-Alaninamide,

RN 222406-88-4 CAPLUS

CN L-.alpha.-Asparagine, N-[(phenylmethoxy)carbonyl]-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dichlorobenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 222406-90-8 CAPLUS

CN Benzoic acid, 2,6-dichloro-,

(3S)-4-carboxy-3-[[[2-(4-fluorophenyl)-6-oxo-

5-[[[(phenylmethyl)amino]carbonyl]amino]-1(6H)-pyrimidinyl]acetyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 222406-92-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-,

(3S)-4-carboxy-3-[[[2-(4-fluorophenyl)-5-[(2furanylcarbonyl)amino]-6-oxo-1(6H)-pyrimidinyl]acetyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 222406-93-1 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[5-[[6-(dimethylamino)-1-

oxohexyl]amino]-2-(4-fluorophenyl)-6-oxo-1(6H)-pyrimidinyl]acetyl]amino]-2oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} F \\ O \\ O \\ O \\ O \end{array}$$

$$\begin{array}{c} C1 \\ O \\ CO_2H \\ O \end{array}$$

$$\begin{array}{c} C1 \\ O \\ CO_2H \\ O \end{array}$$

$$\begin{array}{c} C1 \\ O \\ CO_2H \\ O \end{array}$$

RN 222406-94-2 CAPLUS

CN Benzoic acid, 2,6-dichloro-,

(3S)-4-carboxy-3-[[[2-(4-fluorophenyl)-6-oxo-

5-[(phenylsulfonyl)amino]-1(6H)-pyrimidinyl]acetyl]amino]-2-oxobutyl ester

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 222406-96-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[5-amino-2-(4-fluorophenyl)-6-oxo-1(6H)-pyrimidinyl]acetyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 4 OF 36 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1998:788773 CAPLUS

DOCUMENT NUMBER: 130:66805

TITLE: Preparation of peptide inhibitors of

interleukin-1.beta. converting enzyme

INVENTOR(S): Bemis, Guy W.; Golec, Julian M. C.; Lauffer, David

J.;

Mullican, Michael D.; Murcko, Mark A.; Livingston,

David J.

PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Incorporated, USA

SOURCE: U.S., 106 pp., Cont.-in-part of U.S. 5,656,627.

CODEN: USXXAM

DOCUMENT TYPE:

Patent English

LANGUAGE:

COLDUM: 2

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PA	rent	NO.		KI	ND	DATE			A	PPLI	CATI	ON N	٥.	DATE			
	US	5847	135		A		19981208		U	US 1995-440898				19950525				
	US	5756	466	А			19980526			US 1994-261452								
										US 1995-405581								
	US	5716	929		А		19980210			US 1995-464964				4	19950605			
								WO 1995-US7617										
								BR,										FI.
								ΚE,										
								NZ,										
			TM,		•	·	•	·	•	•	•	·	•		•			
		RW:	KE,	MW,	SD,	SZ,	UG,	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,
								BF,										
					TG				·	•	·	•	•	•	,	•	,	
	CA	2192	089		A	AA 19951228				CA 1995-2192089				39	19950616			
										AU 1995-29446								
								EP 1995-925257										
								ES,										PT,
SE							•	•	,	•	,	•	•			,	,	,
	CN	1159	196		A		1997	0910		Cì	V 19	95-19	94383	L	1995	0616		
		95086					1997	1021		В	R 19	95-8	051		1995	0616		
	HU	76622	2		A2	2	1997	1028		н	J 19	96-3	475		1995	0616		
	ĴΡ	10504	4285		T	2	1998	0428		JI	199	95-50	02478	3	1995	0616		
	NO	10504 96053	365		A		1997	0217		NO	199	96-53	365		1996	1213		
		96050						0214							1996			
PRIO	RITY	APPI	LN.	INFO							199	94-26	51452	2	19940	0617		
										US	199	95-40	05581		19950	0317		
										US	199	95-44	10898	3	1995(0525		
										WC	199	95-US	57617	7	19950	0616		

OTHER SOURCE(S): MARPAT 130:66805

7 175209-21-9P 175209-22-0P 175209-42-4P

175209-46-8P 175209-83-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide inhibitors of interleukin-1.beta. converting enzyme)

RN 175209-21-9 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[[2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyridinyl]acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN175209-22-0 CAPLUS

Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[[2-oxo-3-[(1-oxo-3-CN phenylpropyl)amino]-6-(phenylmethyl)-1(2H)-pyridinyl]acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

175209-42-4 CAPLUS RN

Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[(2S)-2-[(1H-imidazol-2-CN ylcarbonyl)amino]-1-oxopropyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

175209-46-8 CAPLUS RN

Benzoic acid, 2,6-dichloro-,

(3S)-4-carboxy-2-oxo-3-[[(2S)-1-oxo-2-[2-oxo-3-[(1-oxo-3-phenylpropyl)amino]-1(2H)-pyridinyl]propyl]amino]butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

175209-83-3 CAPLUS RN

Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[[(3S)-2,3,4,5-

tetrahydro-2-oxo-5-(1-oxo-3-phenylpropyl)-3-[(1-oxo-3-phenylpropyl)amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 5 OF 36 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER:

1998:568911 CAPLUS

DOCUMENT NUMBER:

129:184238

TITLE:

Screening for thymocyte caspase activity modulators Reinherz, Ellis; Clayton, Linda; Ocain, Timothy D.;

INVENTOR (S):

PATENT ASSIGNEE(S):

Patch, Raymond J. Dana Farber Cancer Institute, USA; Procept, Inc.

PCT Int. Appl., 62 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO. DATE

19980217 WO 1998-US3524 A1 19980820 WO 9836057

W: CA, JP

RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT,

SE

PRIORITY APPLN. INFO.:

US 1997-802474 19970218 19971009 US 1997-948124

191666-52-1P 211918-96-6P 211918-99-9P IT

211919-00-5P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(screening for thymocyte caspase activity modulators)

191666-52-1 CAPLUS RN

L-Valinamide, CN

N-[5-[(3aS, 4S, 6aR)-hexahydro-2-oxo-1H-thieno[3, 4-d]imidazol-4-y1]-l-oxopentyl]-L-.alpha.-aspartyl-L-.alpha.-glutamyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 211918-96-6 CAPLUS

CN L-Alaninamide,

N-[5-[(3aS, 4S, 6aR)-hexahydro-2-oxo-1H-thieno[3, 4-d]imidazol-4-y1]-1-oxopenty1]-L-tyrosyl-L-valyl-N-[(1S)-3-[[2,6bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 211918-99-9 CAPLUS
CN L-Valinamide,
N-[5-[(3aS, 4S, 6aR)-hexahydro-2-oxo-1H-thieno[3, 4-d]imidazol4-yl]-1-oxopentyl]-L-.alpha.-aspartyl-L-.alpha.-glutamyl-N-[(1R)-1-

4-y1]-1-oxopenty1]-L-.alpha.-asparty1-L-.alpha.-glutamy1-N-[(1R)-1-(carboxymethy1)-3-[(2,6-dimethylbenzoy1)oxy]-2-oxopropy1]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 211919-00-5 CAPLUS
CN L-Alaninamide,
N-[5-[(3aS, 4S, 6aR)-hexahydro-2-oxo-1H-thieno[3, 4-d]imidazol4-yl]-1-oxopentyl]-L-tyrosyl-L-valyl-N-[(1R)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

PAGE 1-A

ACCESSION NUMBER:

1998:331708 CAPLUS

DOCUMENT NUMBER:

129:64785

TITLE:

Bimodal Inhibition of Caspase-1 by Aryloxymethyl and

Acyloxymethyl Ketones

AUTHOR(S):

Brady, Kenneth D.

CORPORATE SOURCE:

BASF Bioresearch Corporation, Worcester, MA,

01605-4314, USA

SOURCE:

Biochemistry (1998), 37(23), 8508-8515

CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER:
DOCUMENT TYPE:

American Chemical Society Journal

LANGUAGE:

English

IT 151544-42-2 209055-55-0

RL: BAC (Biological activity or effector, except adverse); BIOL

(Biological study)

(proteinase inhibitor; bimodal inhibition of caspase-1 by

aryloxymethyl

and acyloxymethyl ketones)

RN 151544-42-2 CAPLUS

CN L-Alaninamide,

N-[(phenylmethoxy)carbonyl]-L-valyl-N-[1-(carboxymethyl)-3-

[(2,6-dichlorobenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 209055-55-0 CAPLUS

CN L-Alaninamide,

N-[(phenylmethoxy)carbonyl]-L-valyl-N-[1-(carboxymethyl)-2-oxo-3-(1-oxo-3-phenylpropoxy)propyl]- (9CI) (CA INDEX NAME)

applicant's PCT

```
ANSWER 7 OF 36 CAPLUS COPYRIGHT 1999 ACS
                          1998:251152 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                          128:321926
                          Preparation of aspartate ester inhibitors of
TITLE:
                          interleukin-1.beta. converting enzyme
                          Albrecht, Hans P.; Allen, Hamish John; Brady, Kenneth
INVENTOR(S):
                          Dale; Caprathe, Bradley William; Gilmore, John Lodge;
                          Harter, William Glen; Hays, Sheryl Jeanne; Kostlan,
                          Catherine Rose; Lunney, Elizabeth Ann; Para, Kimberly
                          Suzanne; et al.
                          Warner-Lambert Company, USA; Albrecht, Hans P.;
PATENT ASSIGNEE(S):
Allen,
                          Hamish John; Brady, Kenneth Dale; Caprathe, Bradley
                          William; Gilmore, John Lodge; Harter, William Glen;
                          Hays, Sheryl Jeanne; Kostlan, Catherine Rose
                          PCT Int. Appl., 179 pp.
SOURCE:
                          CODEN: PIXXD2
                          Patent
DOCUMENT TYPE:
                          English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                            APPLICATION NO. DATE
                  KIND DATE
     PATENT NO.
     ___________
     WO 9816502
                                           WO 1997-US18514 19971009
                      A1 19980423
         W: AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ,
MT
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
                      A1 19980511
                                             AU 1997-49023
                                                               19971009
     AU 9749023
                       A1 19990804
                                           EP 1997-911715
                                                               19971009
     EP 932598
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                                             NO 1999-1677
                                                               19990409
                             19990609
     NO 9901677
                     A
                                             US 1996-28322
                                                               19961011
PRIORITY APPLN. INFO.:
                                             WO 1997-US18514 19971009
                          MARPAT 128:321926
OTHER SOURCE(S):
     206863-49-2P 206863-52-7P 206863-53-8P
     206863-54-9P 206863-55-0P 206863-56-1P
     206863-57-2P 206863-58-3P 206863-59-4P
     206863-62-9P 206863-63-0P 206863-64-1P
     206863-65-2P 206863-66-3P 206863-68-5P
     206863-87-8P 206863-89-0P 206863-90-3P
     206863-91-4P 206863-92-5P 206863-93-6P
     206863-94-7P 206863-96-9P 206863-97-0P
     206864-00-8P 206864-01-9P 206864-04-2P
     206864-05-3P 206864-06-4P 206864-07-5P
     206864-08-6P 206864-09-7P 206864-10-0P
     206864-11-1P 206864-12-2P 206864-13-3P
     206864-14-4P 206864-15-5P 206864-16-6P
     206864-17-7P 206864-18-8P 206864-19-9P
```

206864-20-2P 206864-21-3P 206864-22-4P 206864-23-5P 206864-24-6P 206864-25-7P

206864-26-8P 206864-27-9P 206864-28-0P 206864-29-1P 206864-30-4P 206864-31-5P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aspartate ester inhibitors of interleukin-1.beta.

converting

enzyme)

206863-49-2 CAPLUS RN

1-Naphthaleneacetic acid, CN

(3S)-3-[[(2S)-2-(acetylamino)-1-oxopropyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

206863-52-7 CAPLUS RN

1-Naphthaleneacetic acid, 4-carboxy-2-oxo-3-[[1-oxo-2-[(1-oxo-4-CN phenylbutyl)amino]propyl]amino]butyl ester (9CI) (CA INDEX NAME)

206863-53-8 CAPLUS RN

1-Naphthaleneacetic acid, 4-carboxy-3-[[2-[(methylsulfonyl)amino]-1-CN oxopropyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206863-54-9 CAPLUS

1-Naphthaleneacetic acid, 3-[[(2S)-2-[[2-(acetylamino)-1-oxo-4-phenylbutyl]amino]-1-oxopropyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 206863-55-0 CAPLUS
CN 1-Naphthaleneacetic acid,
3-[[2-(acetylamino)-1-oxobutyl]amino]-4-carboxy2-oxobutyl ester (9CI) (CA INDEX NAME)

206863-56-1 CAPLUS RN

1-Naphthaleneacetic acid, 3-[[2-[(5-amino-1,5-dioxopentyl)amino]-1-CN oxopropyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

206863-57-2 CAPLUS RN

1-Naphthaleneacetic acid, 4-carboxy-2-oxo-3-[[1-oxo-2-CN [[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester (9CI) (CA INDEX NAME)

206863-58-3 CAPLUS RN

1-Naphthaleneacetic acid, CN

3-[[2-[(aminocarbonyl)amino]-1-oxopropyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206863-59-4 CAPLUS
CN 1-Naphthaleneacetic acid,
3-[[2-(acetylamino)-1-oxopropyl]amino]-4-carboxy2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206863-62-9 CAPLUS
CN 1-Naphthaleneacetic acid, 3-[[(acetylamino)acetyl]amino]-4-carboxy-2oxobutyl ester (9CI) (CA INDEX NAME)

RN 206863-63-0 CAPLUS
CN Benzenepropanoic acid, .beta.-phenyl-, 3-[[2-(acetylamino)-1-oxopropyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

206863-64-1 CAPLUS RN

L-Alaninamide, N-acetyl-L-.alpha.-glutamyl-N-[1-(carboxymethyl)-3-[(1-CN naphthalenylacetyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

206863-65-2 CAPLUS RN

1-Naphthaleneacetic acid, 4-carboxy-2-oxo-3-[[1-oxo-2-[(1-oxo-3-CN phenylpropyl)amino]propyl]amino]butyl ester (9CI) (CA INDEX NAME)

206863-66-3 CAPLUS ŔŊ

1-Naphthaleneacetic acid, 4-carboxy-3-[[2-[(3-methyl-1-oxobutyl)amino]-1-CN oxopropyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206863-68-5 CAPLUS

CN 1-Naphthaleneacetic acid, 3-[[2-[(aminocarbonyl)amino]-1-oxo-3(phenylmethoxy)propyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \circ \\ \text{H}_2\text{N}-\text{C}-\text{NH} & \text{O} \\ & | & | \\ \text{Ph}-\text{CH}_2-\text{O}-\text{CH}_2-\text{CH}-\text{C}-\text{NH} & \text{O} \\ & | & | & | \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH}-\text{C}-\text{CH}_2-\text{O}-\text{C}-\text{CH}_2 \\ \end{array}$$

RN 206863-87-8 CAPLUS
CN 1-Naphthaleneacetic acid, 4-carboxy-3-[[(3,4-dihydro-1-oxo-2(1H)-isoquinolinyl)acetyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206863-89-0 CAPLUS
CN 2-Naphthaleneacetic acid, 4-carboxy-2-oxo-3-[[(2-oxo-6-phenyl-1-piperidinyl)acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

206863-90-3 CAPLUS RN

1-Naphthaleneacetic acid, 4-carboxy-2-oxo-3-[[(2-oxo-6-phenyl-1-piperidinyl)acetyl]amino]butyl ester (9CI) (CA INDEX NAME) CN

PAGE 1-A

PAGE 2-A

206863-91-4 CAPLUS RN

2-Naphthaleneacetic acid, 1,2,3,4-tetrahydro-1-oxo-, 4-carboxy-3-[[3-CN methyl-1-oxo-2-[(1-oxo-3-phenylpropyl)amino]butyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

206863-92-5 CAPLUS RN ·

2-Naphthaleneacetic acid, 4-carboxy-3-[[(3,4-dihydro-1-oxo-2(1H)-CN isoquinolinyl)acetyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

206863-93-6 CAPLUS RN

Benzenepropanoic acid, .alpha.-(phenylmethyl)-, CN

4-carboxy-3-[[(3,4-dihydro-

1-oxo-2(1H)-isoquinolinyl)acetyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

206863-94-7 CAPLUS RN

Benzenepropanoic acid, .alpha.-(phenylmethyl)-, \cdot CN

4-carboxy-2-oxo-3-[[(2-oxo-

6-phenyl-1-piperidinyl)acetyl]amino]butyl ester (9CI) (CA INDEX NAME)

RN 206863-96-9 CAPLUS

CN 1-Naphthaleneacetic acid, 4-carboxy-3-[[2-(3,4-dihydro-1-oxo-2(1H)-isoquinolinyl)-1-oxopropyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206863-97-0 CAPLUS

CN 2-Naphthaleneacetic acid, 4-carboxy-3-[[2-(3,4-dihydro-1-oxo-2(1H)-isoquinolinyl)-1-oxopropyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206864-00-8 CAPLUS

CN Benzenepropanoic acid, .alpha.-(phenylmethyl)-, 4-carboxy-3-[[2-(3,4-dihydro-1-oxo-2(1H)-isoquinolinyl)-1-oxopropyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206864-01-9 CAPLUS

CN 2-Naphthaleneacetic acid, 1,2,3,4-tetrahydro-1-oxo-,

4-carboxy-3-[[2-(3,4-

dihydro-1-oxo-2(1H)-isoquinolinyl)-1-oxopropyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206864-04-2 CAPLUS

CN 1-Naphthaleneacetic acid, 4-carboxy-2-oxo-3-[[1-oxo-2-(2-oxo-3-phenyl-1-imidazolidinyl)propyl]amino]butyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 206864-05-3 CAPLUS
CN 1-Naphthaleneacetic acid,
4-carboxy-2-oxo-3-[[1-oxo-2-(tetrahydro-2-oxo-3-phenyl-1(2H)-pyrimidinyl)propyl]amino]butyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN

206864-06-4 CAPLUS
1-Naphthaleneacetic acid, 4-carboxy-2-oxo-3-[[(tetrahydro-2-oxo-3-phenyl-1(2H)-pyrimidinyl)acetyl]amino]butyl ester (9CI) (CA INDEX NAME) CN

PAGE 1-A

PAGE 2-A

RN 206864-07-5 CAPLUS
CN 1-Naphthaleneacetic acid,
3-[[2-(acetylamino)-3-methyl-1-oxobutyl]amino]-4carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

O NHAC
$$\begin{matrix} || & || & | \\ || & || & | \\ NH-C-CH-Pr-i & | & | \\ || & | & | \\ HO_2C-CH_2-CH-C-CH_2-O-C-CH_2-CH-CH_2-Ph \\ || & || & || & | \\ || & 0 & O & CH_2-Ph \end{matrix}$$

RN 206864-10-0 CAPLUS
CN Benzenepentanoic acid, .gamma.-(phenylmethyl)-, 3-[[2-(acetylamino)-3-methyl-1-oxobutyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

206864-11-1 CAPLUS RN

2-Naphthaleneacetic acid, 1,2,3,4-tetrahydro-1-oxo-, CN

3-[[2-(acetylamino)-3-

methyl-1-oxobutyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

206864-12-2 CAPLUS

Benzenebutanoic acid, .beta.-(phenylmethyl)-,

4-carboxy-3-[[3-methyl-1-oxo-

2-[(1-oxo-3-phenylpropyl)amino]butyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

206864-13-3 CAPLUS RN

Benzenepropanoic acid, .beta.-phenyl-, 3-[[[3-(acetylamino)-2-oxo-1(2H)-CN pyridinyl]acetyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 206864-15-5 CAPLUS

CN L-Valinamide, N-[(phenylmethoxy)carbonyl]-L-.alpha.-glutamyl-N-[1-(carboxymethyl)-3-[(1-naphthalenylacetyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 206864-16-6 CAPLUS
CN L-Alaninamide,

N-[(phenylmethoxy)carbonyl]-L-valyl-N-[1-(carboxymethyl)-3-[(1-naphthalenylacetyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)